

# Nonlinear Higher-Order Thermo-Hydrodynamics II: Illustrative Examples

J. Galvão Ramos, Áurea R. Vasconcellos, and Roberto Luzzi

*Instituto de Física "Gleb Wataghin",  
Universidade Estadual de Campinas - Unicamp,  
CP 6165, 13083-970, Campinas-SP, Brazil*

(Dated: February 2, 2008)

## Abstract

The construction of a generalized (higher-order) nonlinear thermo-hydrodynamics, based on a nonequilibrium ensemble formalism has been presented in the preceding article. The working of such theory is illustrated in the present one. We consider here the case of two ideal classical fluids in interaction between them, and the nonlinear equations of evolution for the density (a hyperbolic one) and for the velocity field describing motion under flow are derived. Also, now at the quantum level, it is described the nonlinear transport in the fluid of electrons in doped polar semiconductors, and comparison with Monte Carlo calculations and with experimental data is done, obtaining very good agreement.

## I. INTRODUCTION

In the preceding article (hereafter called as I, and when equations present in it are indicated in what follows, we write the number preceded by I) [1], it was described the construction of a generalized (higher-order) and nonlinear thermo-hydrodynamics, based on mechano-statistical foundations. In that way it was established a kind of unification of the microscopic dynamics and a mesoscopic hydrodynamics.

In this follow-up article we attempt to illustrate the functioning of the theory by applying it to a couple of somewhat simplified situations. Both cases are such that we can describe their underlying mechanics in terms of an individuals single-particle approximation. They are: 1. The case of two ideal classical fluids in interaction between them, one being the main system of interest driven away from equilibrium, and the other acting as a thermal reservoir; the associated nonlinear generalized hydrodynamics, however restricted to a study of a first-order one, is derived in section II. 2. A similar case, but now composed of two quantum gases, namely, conduction band electrons in a doped polar semiconductor under the action of an electric field, and the phonon system acting as a thermal bath, is dealt with in section IV. Moreover, the study of section II is complemented in section III with the analysis of diffusion-advection motion governed by a nonlinear hydrodynamic equation.

## II. TWO CLASSICAL FLUIDS IN INTERACTION

Let us consider two ideal classical fluids with interaction between them, with the Hamiltonian given by

$$H = \sum_{j=1}^N \frac{p_j^2}{2m} + \sum_{\mu=1}^{N_R} \frac{P_\mu^2}{2M} + \sum_{j,\mu} \mathcal{V}(|\mathbf{r}_j - \mathbf{R}_\mu|) + V_{ext}, \quad (1)$$

$m$  being the mass of the particles in the system of interest,  $M$  that in the second system taking as a thermal bath at temperature  $T_0$ , and the interaction being of the type of central forces.  $V_{ext}$  stands for the interaction energy with an external source, and it is to be understood that the bath is constantly in equilibrium with an external ideal reservoir. We analyze the *hydrodynamics of this system in a first order approximation*, meaning to take as basic variables of the system of interest the kinetic energy, the density, and the first flux (current)

of the latter, with the associated dynamical quantities being

$$\hat{h}(\mathbf{r}) = \sum_j \frac{p_j^2}{2m} \delta(\mathbf{r} - \mathbf{r}_j), \quad (2)$$

$$\hat{n}(\mathbf{r}) = \sum_j \delta(\mathbf{r} - \mathbf{r}_j), \quad (3)$$

$$\hat{\mathbf{I}}_n(\mathbf{r}) = \sum_j \frac{\mathbf{p}_j}{m} \delta(\mathbf{r} - \mathbf{r}_j), \quad (4)$$

with the understanding that all three are defined in  $\Gamma$ -phase space. The thermal bath is assumed to remain constantly in equilibrium with a reservoir at temperature  $T_0$ , and the system subjected to external forces driving it out of equilibrium.

According to I (the previous article) the auxiliary ("instantaneously frozen") nonequilibrium statistical operator is given by [cf. Eq.(I.6)]

$$\bar{\mathcal{R}}(t, 0) = \bar{\rho}(t, 0) \times \rho_R, \quad (5)$$

where  $\rho_R$  is the canonical distribution at temperature  $T_0$  of the thermal bath, and

$$\bar{\rho}(t, 0) = \exp \left\{ -\phi(t) - \int d^3r \left[ F_h(\mathbf{r}, t) \hat{h}(\mathbf{r}) + A(\mathbf{r}, t) \hat{n}(\mathbf{r}) + \mathbf{F}_n(\mathbf{r}, t) \cdot \hat{\mathbf{I}}_n(\mathbf{r}) \right] \right\}, \quad (6)$$

where, we recall,  $\phi(t)$  ensures the normalization and we have introduced the set of *nonequilibrium thermodynamic variables* (Lagrange multipliers in the variational derivation of the formalism), namely

$$\{F_h(\mathbf{r}, t), A(\mathbf{r}, t), \mathbf{F}_n(\mathbf{r}, t)\}, \quad (7)$$

and we also recall that the nonequilibrium statistical operator is given, in terms of the auxiliary one of Eq.(5), by Eq.(I.4). The corresponding set of *basic hydrodynamic macrovariables* consists of

$$h(\mathbf{r}, t) = \int d\Gamma \hat{h}(\mathbf{r}) \bar{\rho}(t, 0), \quad (8)$$

$$n(\mathbf{r}, t) = \int d\Gamma \hat{n}(\mathbf{r}) \bar{\rho}(t, 0), \quad (9)$$

$$\mathbf{I}_n(\mathbf{r}, t) = \int d\Gamma \hat{\mathbf{I}}_n(\mathbf{r}, t) \bar{\rho}(t, 0), \quad (10)$$

where the integration is over the phase space of the system [cf. Eq.(I.31)]. These equations, Eqs.(8) to (10), are the *nonequilibrium thermodynamic equations of state*, meaning that they relate the basic macrovariables on the left, with the nonequilibrium thermodynamic variables of Eq.(7) present on the right-hand side in the distribution  $\bar{\rho}$  of Eq.(6).

Equations (8) to (10) take the form

$$h(\mathbf{r}, t) = \int d^3p \frac{p^2}{2m} f(\mathbf{r}, \mathbf{p}; t), \quad (11)$$

$$n(\mathbf{r}, t) = \int d^3p f(\mathbf{r}, \mathbf{p}; t), \quad (12)$$

$$\mathbf{I}_n(\mathbf{r}, t) = \int d^3p \frac{\mathbf{p}}{m} f(\mathbf{r}, \mathbf{p}; t), \quad (13)$$

where

$$f(\mathbf{r}, \mathbf{p}; t) = \frac{1}{\mathcal{Z}(t)} \exp \left\{ A(\mathbf{r}, t) - F_h(\mathbf{r}, t) \frac{p^2}{2m} - \mathbf{F}_n(\mathbf{r}, t) \cdot \frac{\mathbf{p}}{m} \right\}, \quad (14)$$

is a Boltzmann-style one-particle distribution function, and

$$\mathcal{Z}(t) = \int d^3r \int d^3p \exp \left\{ A(\mathbf{r}, t) - F_h(\mathbf{r}, t) \frac{p^2}{2m} + \mathbf{F}_n(\mathbf{r}, t) \cdot \frac{\mathbf{p}}{m} \right\}. \quad (15)$$

Performing the calculations we find that

$$n(\mathbf{r}, t) = \frac{N}{\mathcal{Z}(t)} \left( \frac{2\pi m}{F_h(\mathbf{r}, t)} \right)^{3/2} \exp \left\{ A(\mathbf{r}, t) + F_h(\mathbf{r}, t) \frac{1}{2} m v^2(\mathbf{r}, t) \right\}, \quad (16)$$

where we have introduced the barycentric velocity  $\mathbf{v}(\mathbf{r}, t)$  [cf. Eq.(20) below], through the definition (see also Eq.(20) below)

$$\mathbf{F}_n(\mathbf{r}, t) = F_h(\mathbf{r}, t) m \mathbf{v}(\mathbf{r}, t). \quad (17)$$

Moreover, we do find that

$$h(\mathbf{r}, t) = u(\mathbf{r}, t) + n(\mathbf{r}, t) \frac{1}{2} m v^2(\mathbf{r}, t), \quad (18)$$

for the energy, where  $u$  is the internal energy

$$u(\mathbf{r}, t) = \frac{3}{2} \frac{n(\mathbf{r}, t)}{F_h(\mathbf{r}, t)} = \frac{3}{2} n(\mathbf{r}, t) k_B T^*(\mathbf{r}, t), \quad (19)$$

introducing, via the definition  $F_h^{-1} = k_B T^*$ , the field of quasitemperature [2, 3, 4] or nonequilibrium kinetic temperature [5]  $T^*(\mathbf{r}, t)$ , with the last term on the right of Eq.(18) being the drift-kinetic energy, and

$$\mathbf{I}_n(\mathbf{r}, t) = n(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t). \quad (20)$$

It can be noticed that if  $n$  is the concentration of particles, it needs be satisfied the constraint that

$$n = \int d^3r n(\mathbf{r}, t), \quad (21)$$

with  $n(\mathbf{r}, t)$  given by Eq.(12).

Let now go over the generalized hydrodynamic equations, namely those of Eqs.(I.35), (I.36) and (I.38) of I (previous article). We do have that

$$\frac{\partial}{\partial t} h(\mathbf{r}, t) + \nabla \cdot \mathbf{I}_h(\mathbf{r}, t) = J_h(\mathbf{r}, t), \quad (22)$$

where  $\mathbf{I}_h$  is the flux of energy and  $J_h$  is the collision integral;

$$\frac{\partial}{\partial t} n(\mathbf{r}, t) + \nabla \cdot \mathbf{I}_n(\mathbf{r}, t) = 0, \quad (23)$$

which is the conservation equation for the density;

$$\frac{\partial}{\partial t} \mathbf{I}_n(\mathbf{r}, t) + \nabla \cdot I_n^{[2]}(\mathbf{r}, t) = \mathbf{J}_n(\mathbf{r}, t) + \mathbf{F}_{ext}(\mathbf{r}, t), \quad (24)$$

where  $I_n^{[2]}(\mathbf{r}, t)$  is the flux of flux (second-order flux) of particles, namely

$$I_n^{[2]}(\mathbf{r}, t) = \int d\Gamma \sum_j \left[ \frac{\mathbf{p}_j \mathbf{p}_j}{m m} \right] \delta(\mathbf{r} - \mathbf{r}_j) \bar{\rho}(t, 0), \quad (25)$$

with  $[\mathbf{p}_j \mathbf{p}_j]$  standing for tensorial product of vectors, rendering a second-rank tensor,  $\mathbf{F}_{ext}(\mathbf{r}, t)$  stands for external forces [arising out of  $V_{ext}$  in Eq.(1)] applied on the system driven it out of equilibrium, and  $\mathbf{J}_n$  is the collision integral accounting for relaxation processes (towards the thermal bath): See Appendix A. The latter is composed of three contributions: two of them, one introducing a term proportional to the gradient of concentration (and responsible for a perturbational modification of the diffusion effect; cf. Ref.[6]) and another introducing nonlocal effects (correlations in space), are neglected and we conserve the main contribution given by

$$\mathbf{J}_n(\mathbf{r}, t) = - [\Theta_n^{[2]}(\mathbf{r}, t)]^{-1} \mathbf{I}_n(\mathbf{r}, t), \quad (26)$$

introducing the inverse of a second-rank tensor,  $\Theta_n^{[2]}$  having dimension of time and playing the role of a tensorial-in-character Maxwell-relaxation time [4, 7, 8], its explicit expression given in Eq.(A3) of Appendix A.

Finally, to close the system of Eqs.(22) to (24) coupled to the set of Eqs.(16), (18) and (20) - the equations of state - we need to express the second-order flux of Eq.(25) in terms of the basic variables, and we obtain that

$$m I_n^{[2]}(\mathbf{r}, t) = n(\mathbf{r}, t) [k_B T^*(\mathbf{r}, t) 1^{[2]} + m n(\mathbf{r}, t) [\mathbf{v}(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)]] . \quad (27)$$

This second-order flux is related to the field of pressure tensor by

$$P^{[2]}(\mathbf{r}, t) = m I_n^{[2]}(\mathbf{r}, t) - n(\mathbf{r}, t) [\mathbf{v}(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)] = n(\mathbf{r}, t) k_B T^*(\mathbf{r}, t) 1^{[2]} = \frac{2}{3} u(\mathbf{r}, t) 1^{[2]} , \quad (28)$$

after using Eq.(19), recovering the local and instantaneous usual form of the hydrostatic pressure.

This first-order hydrodynamics of this simple modeled system sets clearly in evidence the *nonlinearity* referred to in I, namely, one coming out of the expression for the second flux, cf. Eq.(27), and other the higher nonlinear expression for the collision integrals. We also stress that in Eq.(26)  $\Theta_n^{[2]}(\mathbf{r}, t)$  is also highly nonlinear in the basic thermodynamic variables.

In that way it has been explicitly shown that nonlinearities are always present in the generalized hydrodynamic equations, and we further illustrate the matter first, on the basis of the results above, deriving nonlinear equations of evolution for the density and the velocity in the fluid under flow, and after that a study of electric current in a system of mobile electrons in a doped polar semiconductor, dealt with at the quantum mechanical level.

### III. NONLINEAR EQUATIONS OF EVOLUTION

Let us consider the equations of evolution for the basic variables of Eqs.(8) to (10), given by Eqs.(22), (23) and (24). Deriving in time Eq.(23) and using Eq.(24) it follows that

$$\frac{\partial^2}{\partial t^2} n(\mathbf{r}, t) = -\nabla \cdot \frac{\partial}{\partial t} \mathbf{I}_n(\mathbf{r}, t) = \nabla \cdot \nabla \cdot I_n^{[2]}(\mathbf{r}, t) + \nabla \cdot \frac{\mathbf{I}_n(\mathbf{r}, t)}{\Theta_n(\mathbf{r}, t)} - \nabla \cdot \mathbf{F}_{ext}(\mathbf{r}, t) , \quad (29)$$

where for simplicity we have taken the tensorial Maxwell characteristic time of Eq.(26) as a scalar (see Appendix A).

Equation (29) can be rewritten as

$$\begin{aligned} \Theta_n(\mathbf{r}, t) \frac{\partial^2}{\partial t^2} n(\mathbf{r}, t) + \frac{\partial}{\partial t} n(\mathbf{r}, t) + \nabla \cdot [n(\mathbf{r}, t) \mathbf{v}_a(\mathbf{r}, t)] = \\ \Theta_n(\mathbf{r}, t) \nabla \cdot \nabla \cdot I_n^{[2]}(\mathbf{r}, t) - \Theta_n(\mathbf{r}, t) \mathbf{I}_n(\mathbf{r}, t) \cdot \nabla \Theta_n^{-1}(\mathbf{r}, t), \end{aligned} \quad (30)$$

after multiplying by  $\Theta$  and the definition

$$\Theta_n(\mathbf{r}, t) \nabla \cdot \mathbf{F}_{ext}(\mathbf{r}, t) \equiv \nabla \cdot [n(\mathbf{r}, t) \mathbf{v}_a(\mathbf{r}, t)], \quad (31)$$

introducing  $\mathbf{v}_a$  which we call velocity responsible for creating a driven flow in the system.

Second, in order to close Eq.(30) we need to express the second-order flux in terms of the basic variables,  $n$  and  $\mathbf{I}_n$ , which after some calculus takes the form

$$I_n^{[2]}(\mathbf{r}, t) = n(\mathbf{r}, t) k_B T^*(\mathbf{r}, t) 1^{[2]} + n(\mathbf{r}, t) [\mathbf{v}(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)]. \quad (32)$$

Using this Eq.(32) in Eq.(30) and, for further simplifying the presentation, let us take  $\Theta_n(\mathbf{r}, t)$  as smoothly dependent on  $\mathbf{r}$  and  $t$ , i.e. its gradient and time derivative can be neglected, we finally obtain that

$$\begin{aligned} \Theta_n(\mathbf{r}, t) \frac{\partial^2}{\partial t^2} n(\mathbf{r}, t) + \frac{\partial}{\partial t} n(\mathbf{r}, t) - \mathcal{D}_n(\mathbf{r}, t) \nabla^2 n(\mathbf{r}, t) = \\ -\nabla \cdot [n(\mathbf{r}, t) \mathbf{v}_a(\mathbf{r}, t)] + \Theta_n(\mathbf{r}, t) \nabla \cdot \nabla \cdot \left( n(\mathbf{r}, t) [\mathbf{v}(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)] \right) + G_n(\mathbf{r}, t), \end{aligned} \quad (33)$$

where  $G_n$  contains gradients and time derivatives of  $\Theta_n(\mathbf{r}, t)$  which, for simplicity we ignore in what follows,

$$\mathcal{D}_n(\mathbf{r}, t) = \frac{1}{3} v^2(\mathbf{r}, t) \Theta_n(\mathbf{r}, t), \quad (34)$$

we have used that  $\mathbf{I}_n(\mathbf{r}, t) = n(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)$ , and the second contribution on the right-hand side - arising out of the contribution of the so-called convective pressure - can be written as

$$\begin{aligned} \nabla \cdot \nabla \cdot \left( n(\mathbf{r}, t) [\mathbf{v}(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)] \right) = & \left( \mathbf{v}(\mathbf{r}, t) \cdot \nabla \right)^2 n(\mathbf{r}, t) + 2 \left( \mathbf{v}(\mathbf{r}, t) \cdot \nabla n(\mathbf{r}, t) \right) \nabla \cdot \mathbf{v}(\mathbf{r}, t) \\ & + n(\mathbf{r}, t) \left( \nabla \cdot \mathbf{v}(\mathbf{r}, t) \right)^2 + 2 n(\mathbf{r}, t) \left( \mathbf{v}(\mathbf{r}, t) \cdot \nabla \right) \left( \nabla \cdot \mathbf{v}(\mathbf{r}, t) \right) \\ & + n(\mathbf{r}, t) \tilde{\Lambda}^{[2]}(\mathbf{r}, t) \otimes \tilde{\Lambda}^{[2]}(\mathbf{r}, t) \\ & + \left[ \mathbf{v}(\mathbf{r}, t) : \nabla n(\mathbf{r}, t) \right] \otimes \tilde{\Lambda}^{[2]}(\mathbf{r}, t), \end{aligned} \quad (35)$$

where  $\tilde{\Lambda}^{[2]}$  is the velocity-gradient tensor,  $\tilde{\Lambda}^{[2]} = [\nabla \mathbf{v}(\mathbf{r}, t)]$ .

Hence, the equation of evolution for the density, Eq.(3), is dependent on the velocity field and then it needs be coupled to the equation of evolution for the velocity, which is

$$n(\mathbf{r}, t) \left[ \frac{\partial}{\partial t} + \mathbf{v}(\mathbf{r}, t) \cdot \nabla \right] \mathbf{v}(\mathbf{r}, t) = -\frac{1}{m} \nabla \cdot P^{[2]}(\mathbf{r}, t) - n(\mathbf{r}, t) \frac{\mathbf{v}(\mathbf{r}, t) - \mathbf{v}_a(\mathbf{r}, t)}{\tau_n(\mathbf{r}, t)}, \quad (36)$$

where the pressure tensor field is given by  $P^{[2]}(\mathbf{r}, t) = n(\mathbf{r}, t) k_B T^*(\mathbf{r}, t) \mathbf{1}^{[2]}$ .

Equation (33) is a nonlinear Maxwell-Cattaneo-like equation with sources. Moreover, in the strong condition of neglecting the right-hand side and the second derivative in time implying in a movement in conditions such that  $\omega \Theta_n \ll 1$ , we recover the standard Fick's diffusion equation

$$\frac{\partial}{\partial t} n(\mathbf{r}, t) - \mathcal{D}_n(\mathbf{r}, t) \nabla^2 n(\mathbf{r}, t) = 0. \quad (37)$$

Next let us introduce the effects of advection in the diffusive regime, i.e. the density follows the diffusion-advection equation of evolution, as given by Eq.(33), in the condition  $\omega \Theta_n \ll 1$  (thus neglecting the second derivative in time), and for simplicity we illustrate the matter in the case of motion restricted to proceed in  $x$ -direction; hence we do have that

$$\frac{\partial}{\partial t} n(x, t) - \mathcal{D}_n(x, t) \frac{\partial^2}{\partial x^2} n(x, t) = -\frac{\partial}{\partial x} [n(x, t) v_a(x, t)] + \Theta_n(x, t) \frac{\partial^2}{\partial x^2} [n(x, t) v^2(x, t)] \quad (38)$$

Moreover, the diffusion coefficient has the standard expression of kinetic theory (in one dimension),  $\mathcal{D}_n = v_{th}^2 \Theta_n$ , where  $v_{th}$  is the local and instantaneous thermal velocity  $m v_{th}^2(x, t) = k_B T^*(x, t)$ .

Equation (38) can be reorganized in the following way:

$$\begin{aligned} \frac{\partial}{\partial t} n(x, t) - \mathcal{D}_n(x, t) \frac{\partial^2}{\partial x^2} n(x, t) = & -\frac{\partial}{\partial x} [n(x, t) v_a(x, t)] + 2 \Theta_n(x, t) n(x, t) v(x, t) \frac{\partial^2 v^2(x, t)}{\partial x^2} \\ & + 2 \Theta_n(x, t) n(x, t) \left[ \frac{\partial v(x, t)}{\partial x} \right]^2 + 2 \Theta_n(x, t) v(x, t) \frac{\partial}{\partial x} n(x, t) \frac{\partial}{\partial x} v(x, t), \end{aligned} \quad (39)$$

where

$$\mathcal{D}_n(x, t) = \Theta_n(x, t) [v_{th}^2(x, t) + v^2(x, t)], \quad (40)$$

that is, a diffusion coefficient whose standard kinetic theory expression is modified adding to the contributions of the thermal velocity the one of the drift velocity. This contribution together with the last three on the right-hand side of Eq.(39) have their origin in the second divergence of the convection pressure, and it can be noticed that all are nonlinear (quadratic)



in  $v(x, t)$ . The first term on the right of Eq.(39), we recall, is related to the divergence of the driving force producing the advective motion [cf. Eq.(31)].

Moreover, as already noticed, Eq.(39) needs be solved in conjunction with the equation of evolution for the velocity, in this case of motion under flow given by

$$n(x, t) \frac{\partial}{\partial t} v(x, t) + n(x, t) v(x, t) \frac{\partial}{\partial x} v(x, t) = - \frac{k_B}{m} \frac{\partial}{\partial x} T^*(x, t) n(x, t) - n(x, t) \Theta_n^{-1}(x, t) [v(x, t) - v_a(x, t)] , \quad (41)$$

where we used that  $p(x, t) = n(x, t) k_B T^*(x, t)$ .

#### IV. NONLINEAR QUANTUM TRANSPORT IN SEMICONDUCTORS

We consider the case of polar semiconductors described by a two-inverted-parabolic bands model (in the effective mass approximation and conduction band secondary valleys are ignored), where a concentration  $n_e$  of mobile electrons in the conduction band has been created by doping. A constant electric field of intensity  $E_0$  in, say,  $x$ -direction is applied, which accelerates the electrons ("hot" electrons) while there follows a transferring of their energy and momentum (in excess of equilibrium) to the phonon field. The sample is in contact with a thermal reservoir at temperature  $T_0$ , with the phonons being warmed up in scattering events involving Fröhlich, deformation potential, and piezoelectric interactions with the "hot" electrons [9, 10] (see also Ch. 6 in the book of Ref.[11]). Scattering by impurities is neglected in comparison with the one due to lattice vibrations. Moreover, in these polar semiconductors of the different types of electron-phonon interaction we keep only the predominant Fröhlich (polar) interaction.

The electric field  $\mathbf{E}$  creates a (uniform in space) current, that is, a flux of charged particles, and then we have a kind of hydrodynamic motion of the like of the one analysed in the previous sections, except that, as noticed, the hydrodynamic variables are uniform in space (independent of position  $\mathbf{r}$ ), and the thermal bath is played by the phonons. We resort to a first-order hydrodynamics, as in section II, namely, we consider the carriers' energy, the density of particles and the flux of particles. The latter multiplied by the effective mass of the conduction band electrons is the linear momentum, and while the density of particles remains constant in time, as noticed the energy and the momentum change in time. The Hamiltonian is composed of the energies of the electrons in the conduction band (treated as

usual in the random-phase approximation thus including Coulomb interaction in a mean-field approximation) and that of the polar (longitudinal optical) phonons, we call  $\hat{H}_0$  this part, plus the Fröhlich interaction of electrons and polar phonons and the interaction of the electrons with the electric field, we call  $\hat{H}'$  this part. Moreover, differently in other aspect with the case of section II we need here to use a quantum approach.

Taking as basic dynamical variables  $\hat{H}_e$ ,  $\hat{H}_{LO}$ ,  $\hat{N}$ ,  $\hat{\mathbf{P}}$  (energy of electrons  $\hat{H}_e$  and polar phonons  $\hat{H}_{LO}$ , number of electrons, and linear momentum of the electrons) the auxiliary ("instantaneously frozen") statistical operator is then given by

$$\bar{\rho}(t, 0) = \exp \left\{ -\phi(t) - \beta(t) \left[ \hat{H}_e - \mu(t) \hat{N} - \mathbf{v}(t) \cdot \hat{\mathbf{P}} \right] - \beta_{LO}(t) \hat{H}_{LO} \right\} \rho_R, \quad (42)$$

where, we recall,  $\phi(t)$  ensures the normalization condition, and we have introduced the nonequilibrium thermodynamic variables

$$\left\{ \beta(t) \equiv 1/k_B T^*(t), -\beta(t) \mu(t), -\beta(t) \mathbf{v}(t), \beta_{LO}(t) \equiv 1/k_B T_{LO}^*(t) \right\}, \quad (43)$$

interpreted as nonequilibrium quasitemperature,  $T^*$ , quasi-chemical potential,  $\mu$ , and drift velocity,  $\mathbf{v}$ , of the electrons, and quasitemperature of the polar phonons,  $T_{LO}^*$ . Finally,  $\rho_R$  is the statistical operator of the reservoir at temperature  $T_0$ .

We call the basic macrovariables

$$\left\{ E_e(t), N, \mathbf{P}(t), E_{LO}(t) \right\}, \quad (44)$$

where  $N$  is constant in time, and we recall, the density is indicated by  $n$ , and the nonequilibrium thermodynamic equations of state are, after direct calculation, given by

$$\frac{1}{V} E_e(t) = \frac{3}{2} n k_B T^*(t) + \frac{1}{2} n m^* v^2(t), \quad (45)$$

$$\frac{1}{V} \mathbf{P}(t) = n m^* \mathbf{v}(t), \quad (46)$$

$$\frac{1}{V} E_{LO}(t) = \frac{1}{V_{cell}} \hbar \omega_0 \left[ \exp \{ \beta_{LO}(t) \hbar \omega_0 \} - 1 \right]^{-1}, \quad (47)$$

where, 1. In the conditions of concentration and values of quasitemperature involved in the applications, the nonequilibrium time-dependent Fermi-Dirac-like distribution of the internally thermalized electrons in band states in the effective mass approximation can be

approximated by a nonequilibrium time-dependent Boltzmann-Maxwell one [9, 11], and then there follows the first term on the right of Eq.(45), namely, equipartition at each time  $t$  in terms of the quasitemperature  $T^*(t)$  of the "hot" electrons of effective mass  $m^*$ , and the other term is evidently the kinetic energy of drift (current). 2. The polar phonons have been treated in a dispersionless approximation (Einstein model), with unique frequency  $\omega_0$ ,  $V_{cell}$  is the volume of the unit cell in the crystal, and  $V$  is the volume of the sample.

On the other hand the equations of evolution (see Appendix B) are

$$\frac{d}{dt}E_e(t) = \frac{e}{m^*}\mathbf{E} \cdot \mathbf{P}(t) - |J_E(t)|, \quad (48)$$

for the energy of the electrons,

$$\frac{d}{dt}\mathbf{P}(t) = e n \mathbf{E} - |\mathbf{J}_P(t)|, \quad (49)$$

for the electron linear momentum in the direction of the applied field,

$$\frac{d}{dt}E_{LO}(t) = |J_P(t)| - |J_{an}(t)|, \quad (50)$$

for the energy of the polar phonons; volume  $V$  has been taken as 1.

In Eq.(48) the first term on the right accounts for the pumping of energy on the carrier system because of the presence of the electric field, while the second represents the rate of excess energy transferred to the polar phonons. In Eq.(49) the first term on the right is the force produced by the presence of the electric field, and the second the rate of momentum transferred to the lattice. In Eq.(50) the first term on the right is the gain of energy pumped on the phonons by the nonequilibrated ("hot") carriers, with the second being the transfer - via anharmonic processes - of such energy to the acoustic phonons acting as a thermal bath (finally, from the latter there follows a transfer to the thermal reservoir). As noticed, their expressions are given in the Appendix B with the calculations being performed in the Markovian [24, 25, 26]. We write down here the two collision integrals of Eqs.(48) and (49) to illustrate the *highly nonlinear dependence* of them on the nonequilibrium thermodynamic variables,  $\beta(t)$  and  $\mathbf{v}(t)$ , which, on the other hand, are related to the basic variables through the also *nonlinear equations of state*, viz. Eqs.(45) and (46):

$$|J_E(t)| = \mathcal{A}_E y^{3/2} e^{-x} n \left[ \nu_0 A_1 - (\nu_0 + 1) A_2 \right], \quad (51)$$

$$|J_P(t)| = \mathcal{A}_P y^{3/2} e^{-x} n \left[ \nu_0 A_3 - (\nu_0 + 1) A_4 \right], \quad (52)$$

where

$$y(t) = \beta(t) \hbar \omega_0 \quad ; \quad x(t) = \frac{1}{2} m^* v^2(t) / k_B T^*(t), \quad (53)$$

$$\mathcal{A}_E = \left( \frac{2 \hbar \omega_0}{\pi m^*} \right)^{1/2} e \mathcal{E}_0 \quad ; \quad \mathcal{A}_P = \frac{e \mathcal{E}_0}{2\sqrt{\pi}}, \quad (54)$$

$$\nu_0 = \left[ \exp \{ \beta_{LO}(t) \hbar \omega_0 \} - 1 \right]^{-1}, \quad (55)$$

$$A_1(t) = \frac{e^{y/2}}{y} K_0(y/2) + \sum_{n=1}^{\infty} \frac{(4xy)^n}{(2n+1)!} (-1)^n \frac{d^n}{dy^n} \left[ \frac{e^{y/2}}{y} K_0(y/2) \right], \quad (56)$$

$$A_2(t) = e^{-y} \frac{e^{y/2}}{y} K_0(y/2) + \sum_{n=1}^{\infty} \frac{(4xy)^n}{(2n+1)!} (-1)^n \frac{d^n}{dy^n} \left[ \frac{e^{y/2}}{y} K_0(y/2) \right], \quad (57)$$

$$\begin{aligned} A_3(t) = & \frac{1}{3} (4xy)^{1/2} \frac{e^{y/2}}{y} \left[ K_0(y/2) - K_1(y/2) \right] \\ & + \sum_{n=2}^{\infty} \frac{2n}{(2n+1)!} (4xy)^{\frac{2n-1}{2}} (-1)^{n-1} \frac{d^{n-1}}{dy^{n-1}} \left[ \frac{e^{y/2}}{y} \left( K_0(y/2) - K_1(y/2) \right) \right], \end{aligned} \quad (58)$$

$$\begin{aligned} A_4(t) = & \frac{1}{3} e^{-y} (4xy)^{1/2} \frac{e^{y/2}}{y} \left[ K_0(y/2) + K_1(y/2) \right] \\ & + \sum_{n=2}^{\infty} \frac{2n}{(2n+1)!} (4xy)^{\frac{2n-1}{2}} (-1)^{n-1} \frac{d^{n-1}}{dy^{n-1}} \left[ \frac{e^{y/2}}{y} \left( K_0(y/2) + K_1(y/2) \right) \right]. \end{aligned} \quad (59)$$

In these expressions - and note that we have omitted on the right-hand side to explicitly indicate the dependence on time of the different quantities involved -  $K_n$  stands for Bessel function of order  $n$  [12] and  $\mathcal{E}_0$  is the Fröhlich field intensity in the polar interaction [13].

It is worth noticing that in quantities  $A_3$  and  $A_4$  [cf. Eqs.(58) and (59)] it can be put in evidence the quantity  $x^{1/2}$  which is proportional to  $v$ , and therefore we can formally write Eq.(49) as

$$\frac{d}{dt} v(t) = \frac{e}{m^*} E_0 - \frac{v(t)}{\tau_p(t)}, \quad (60)$$

after using Eq.(46), being an equation of the Newton-Langevin type but where  $\tau_p(t)$  plays the role of a relaxation time of the velocity (momentum) which is depending on time through

its dependence on the nonequilibrium thermodynamic state of the system, i.e. depends on a highly nonlinear way on  $\beta(t)$ ,  $\beta_{LO}(t)$ , and the velocity  $v(t)$ . Equation (60) can be alternatively written in the form of the integral equation

$$v(t) = \frac{e}{m^*} E_0 \tau_c(t), \quad (61)$$

where

$$\tau_c(t) = \exp \{-\psi(t)\} \int_0^\infty dt' \exp \{\psi(t')\}, \quad (62)$$

with

$$\psi(t) = \int_0^t dt' \tau_P^{-1}(t'), \quad (63)$$

after taking into account the initial condition  $v(0) = 0$ . Moreover, once the current density is given by

$$I(t) = e n v(t), \quad (64)$$

using Eq.(61) we can write

$$I(t) = \sigma(t) E_0, \quad (65)$$

introducing a time-dependent (on the evolution of the nonequilibrium thermodynamic state of the system) Drude-type conductivity

$$\sigma(t) = \frac{n e^2}{m^*} \tau_c(t). \quad (66)$$

Next we illustrate numerically the matter considering the polar semiconductor GaAs and the strong polar ones and large gap GaN (of present interest for its use in blue diodes and lasers [14]). Figure 1 shows the increase, in the steady state (which follows after a transient of a few picoseconds), of the electrons' quasitemperature with the electric field strength in the case of doped ( $n \simeq 10^{16} cm^{-3}$ ) GaAs at a reservoir temperature  $T_0 = 300K$ . The dots are the result of a Nonequilibrium Molecular Dynamics (Monte Carlo-style) simulation (from Ref.[15]), where we can see a good agreement between both types of approaches.

In Figure 2 are displayed the results of the calculations of the electrons' mobility (left ordinate) in the steady state of doped ( $n \simeq 5 \times 10^{15} cm^{-3}$ ) GaAs, as well as the momentum

relaxation time (right ordinate), in the Ohmic regime, as a function of the reservoir temperature: It can be noticed a good agreement with the experimental data taken from three sources, namely, Refs.[16], [17] and [18].

Going over the particular case of the large-gap strongly polar GaN (in the cubic, i.e. zincblende, phase with  $n \simeq 10^{18} cm^{-3}$ , and  $T_0 = 300K$ ), we can see in Figure 3 the increase of the electron-drift velocity with the electric field intensity, and a good agreement can be noticed in a comparison with the NMD-Monte Carlo simulation, the dots, taken from Ref.[19].

Finally, in Figure 4 we can accompany the evolution in time of the electron-drift velocity in doped ( $n \simeq 10^{17} cm^{-3}$ ) cubic GaN, where in the horizontal axis we do have the travelled distance at any time  $t$ , i.e.  $v t$ , and in the presence of an electric field intensity of  $30KV/cm$ . We can notice, first, that the transient time is roughly of the order of 300 femtoseconds and it can be observed the presence of a so-called "velocity overshoot" at roughly 100 femtoseconds. The agreement with the NDM-Monte Carlo simulation, of Ref.[20], is very good. The calculations and figures are from Ref.[21].

## V. CONCLUDING REMARKS

As noticed in the Introduction, in the previous article in this issue it was described the construction of a generalized higher-order-nonlinear hydrodynamics based on a nonequilibrium ensemble formalism. This means a mechano-statistical foundation in terms of a generalized nonequilibrium grand-canonical ensemble, in that way establishing a kind of unification of the microscopic dynamics and a mesoscopic hydrodynamics. In this follow up article we present some illustrations on the working of the formalism. In Section II we have considered the case of a system composed of two ideal fluids in interaction between them. It is used a truncated hydrodynamic description in which are included solely the density of energy, the density of particles, and the first flux (current) of particles. As discussed elsewhere this implies on restrictions on the characteristics of the hydrodynamic motion, basically the case of those restricted to long to intermediate wavelengths [6, 22], i.e. a hydrodynamics of first order. The continuity equations are derived [cf. Eqs.(22) to (24)] and to close them, in this truncated description, one needs to express the second-order flux in Eq.(24) in terms of the basic variables. In doing this we find a first source of nonlinearity as can be seen in

Eq.(27). Moreover, the collision integrals on the right of these equations of evolution are highly nonlinear as shown, for the case of the one in the equation of evolution for the first flux, in Appendix A in the model of two ideal fluids in interaction, and in Appendix B for the case of a fluid of conduction electrons in doped semiconductors. In the first case the collision integral is composed of several contributions: One dependent on the gradient of the density, as it should appear in a mesoscopic hydrodynamics of this type [23]. Other accounting for nonlocal effects, and a local in space third one which is of the type of Maxwell's contribution [4, 7, 8]; cf. Eq.(A6). It is of a tensorial (rank 2) character and highly nonlinear in the nonequilibrium thermodynamic variables, and then dependent on the position and time.

Section III deals with the motion under flow (advective motion) for the case of the description of Section II. The equations of evolution for the density of particles and for the field of velocity - which are coupled - are obtained. In that way are derived, respectively, a generalized Maxwell-Cattaneo-type equation and a generalized Navier-Stokes-like equation. The nonlinearities are present, and the generalized diffusion coefficient is dependent on the local and instantaneous nonequilibrium thermodynamic state of the system.

Finally, in Section IV it is considered quantum transport in doped polar semiconductors, that is we deal with the homogenous current of the mobile electrons. In this case it is obtained in the steady state - that sets in after a very short (nanosecond scale) transient - when under the action of a constant electric field (that is, the space dependence carried on in the previous Sections is not present). It is derived the dependence of the nonequilibrium electron temperature (carrier's quasitemperature) on the electric field intensity as well as of the drift velocity (the current is proportional to it) in several cases: Comparison with computational modeling Monte Carlo calculations and with experimental data is done following a very good agreement.

## Acknowledgments

We acknowledge financial support from São Paulo State Research Foundation (FAPESP). ARV and RL are Brazil National Research Council (CNPq) research fellows.

## APPENDIX A: THE COLLISION INTEGRAL

The collision integral present on the right-hand side of Eq.(17), resulting from the collisions of the two types of particles via the potential  $\mathcal{V}(|\mathbf{r}_j - \mathbf{R}_\mu|)$  [cf. Eq.(1)] is given in the Markovian approximation [11, 24, 25, 26] by the expression

$$\mathbf{J}_n(\mathbf{r}, t) \simeq \int_{-\infty}^0 dt' e^{\epsilon(t'-t)} \int d\Gamma \left\{ \hat{H}'(\Gamma|t' - t)_0, \left\{ \hat{H}'(\Gamma), \hat{\mathbf{I}}_n(\Gamma|\mathbf{r}) \right\} \right\} \bar{\rho}(t, 0) \times \rho_R, \quad (\text{A1})$$

where  $\hat{H}'(t' - t)_0$  indicates evolution under the dynamics generator by  $\hat{H}_0$  - i.e. in the interaction representation -, and we use for the statistical distribution of the reservoir,  $\rho_R$ , a canonical one with temperature  $\beta_R$ . It can be noticed that the approximate (Markovian) scattering integral of Eq.(A1) is quadratic in the interaction strength and corresponds in the classical limit to the Golden Rule of Quantum Mechanics, and we recall that  $\{\dots, \dots\}$  stands for Poisson bracket.

The lengthy but straightforward calculation of Eq.(1) provides several contributions to this scattering integral: one involving the gradient of the concentration (leading to a correction (renormalization) of the diffusion coefficient due to the collisions), other involving the gradient of the quasitemperature (implying in a cross-effect between thermal and material motion). Another one is related to introduce correlation effects in space of the collisional processes (i.e. nonlocal effects). Finally, the most relevant contribution is given by

$$\mathbf{J}_n(\mathbf{r}, t) \simeq -\frac{N_R}{m m_r V^2} \sqrt{\frac{\pi}{2}} (M \beta_R)^{3/2} \sum_{\mathbf{q}} \frac{|\mathcal{V}(q)|^2}{q} [\mathbf{q} \mathbf{q}] \mathbf{A}(\mathbf{r}, \mathbf{q}), \quad (\text{A2})$$

where

$$\mathbf{A}(\mathbf{r}, \mathbf{q}) = n(\mathbf{r}, t) \left[ \frac{\beta(\mathbf{r}, t)}{2\pi m} \right]^{3/2} \int d^3 p \mathbf{p} \exp \left\{ -\frac{\beta(\mathbf{r}, t)}{2m} [\mathbf{p} - m \mathbf{v}(\mathbf{r}, t)]^2 - \frac{M \beta_R}{2m^2 q^2} (\mathbf{q} \cdot \mathbf{p})^2 \right\} \quad (\text{A3})$$

In Eqs.(A2) and (A3),  $\mathcal{V}(\mathbf{q})$  is the Fourier transform of the interaction potential between the two types of particles,  $m_r$  is the reduced mass,  $m_r^{-1} = m^{-1} + M^{-1}$ , and  $N_R$  is the number of particles in the thermal bath.

Introducing a shift in coordinate  $\mathbf{p}$ , namely

$$\mathbf{p} = \mathbf{P} + \mathbf{b}, \quad (\text{A4})$$

with

$$\left[ \beta(\mathbf{r}, t) 1^{[2]} + \frac{M \beta_R}{m q^2} [\mathbf{q} \mathbf{q}] \right] \mathbf{b}(\mathbf{r}, t) = \beta m \mathbf{v}(\mathbf{r}, t), \quad (\text{A5})$$



and performing the calculations we arrive at the result that

$$\mathbf{J}_n(\mathbf{r}, t) \simeq [\Theta_n^{[2]}(\mathbf{r}, t)]^{-1} \mathbf{I}_n(\mathbf{r}, t), \quad (\text{A6})$$

where  $\Theta$  is a rank-two tensor with dimensions of time, playing the role of a tensorial Maxwell-relaxation time [4, 7, 8], with its inverse given by

$$[\Theta_n^{[2]}(\mathbf{r}, t)]^{-1} = -\frac{n_R \beta_R}{m} \frac{m + M}{m} \left( \frac{\pi M \beta_R}{2} \right)^{1/2} \left[ \frac{m \beta(\mathbf{r}, t)}{m \beta(\mathbf{r}, t) + M \beta_R} \right]^{3/2} K^{[2]}(\mathbf{r}, t), \quad (\text{A7})$$

where

$$K^{[2]}(\mathbf{r}, t) = \frac{1}{V} \sum_{\mathbf{q}} |\mathcal{V}(q)|^2 \frac{[\mathbf{q} \mathbf{q}]}{q} \exp \left\{ -\frac{m M \beta_R \beta(\mathbf{r}, t)}{2 [m \beta(\mathbf{r}, t) + M \beta_R]} \frac{(\mathbf{q} \cdot \mathbf{v}(\mathbf{r}, t))^2}{q^2} \right\}, \quad (\text{A8})$$

with  $n_R$  being the density of particles in the thermal bath.

We stress that this tensorial Maxwell-relaxation time depends on position and time through its dependence on the basic nonequilibrium thermodynamic variables  $\beta(\mathbf{r}, t)$  and  $\mathbf{v}(\mathbf{r}, t)$ : recalling that  $\mathbf{I}_n(\mathbf{r}, t) = n(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)$ , this time-relaxation-type contribution is not a linear one, but a highly nonlinear in  $\mathbf{v}(\mathbf{r}, t)$ . In fact, performing the integration in Eq.(A8) we find that  $K_{ij} = 0$  for  $i \neq j$ , and there survive the diagonal terms

$$K_{xx}(\mathbf{r}, t) = K_{yy}(\mathbf{r}, t) = \xi(0) \Phi \left( \frac{m}{2} \tilde{\beta}(\mathbf{r}, t) v^2(\mathbf{r}, t) \right) - \frac{1}{2} K_{zz}(\mathbf{r}, t), \quad (\text{A9})$$

$$K_{zz}(\mathbf{r}, t) = \xi(0) \left[ \frac{m}{2} \tilde{\beta}(\mathbf{r}, t) v^2(\mathbf{r}, t) \right]^{-3/2} \gamma \left( \frac{3}{2}, \frac{m}{2} \tilde{\beta}(\mathbf{r}, t) v^2(\mathbf{r}, t) \right), \quad (\text{A10})$$

where

$$\tilde{\beta}(\mathbf{r}, t) = \frac{M \beta_R \beta(\mathbf{r}, t)}{m \beta(\mathbf{r}, t) + M \beta_R}, \quad (\text{A11})$$

$$\Phi \left( \frac{m}{2} \tilde{\beta}(\mathbf{r}, t) v^2(\mathbf{r}, t) \right) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{2}{(2k-1)(k-1)!} \left( \frac{m}{2} \tilde{\beta}(\mathbf{r}, t) v^2(\mathbf{r}, t) \right)^{2(k-1)}, \quad (\text{A12})$$

$$\xi(0) = \frac{1}{8 \pi^2} \int_0^{q_0} dq q^3 |\mathcal{V}(\mathbf{q})|^2, \quad (\text{A13})$$

with  $q_0$  being a cut-off limit of the order of the inverse of the mean distance between particles of the system and the bath,  $\gamma$  is the incomplete Gamma function [12], and we can also alternatively write

$$K_{zz}(\mathbf{r}, t) = \xi(0) \sum_0^{\infty} (-1)^k \frac{2}{(k + \frac{3}{2}) k!} \left( \frac{m}{2} \tilde{\beta}(\mathbf{r}, t) v^2(\mathbf{r}, t) \right)^k. \quad (\text{A14})$$

It may be noticed that we can write

$$[\Theta_n^{[2]}(\mathbf{r}, t)]^{-1} = \frac{1^{[2]}}{\Theta_n(\mathbf{r}, t)} + \left[ \overset{\circ}{\Theta}_n^{[2]}(\mathbf{r}, t) \right]^{-1}, \quad (\text{A15})$$

where

$$\frac{1}{\Theta_n(\mathbf{r}, t)} = \frac{1}{3} \text{Tr} \left\{ [\Theta_n^{[2]}(\mathbf{r}, t)]^{-1} \right\}, \quad (\text{A16})$$

and the last term is then traceless, and accounting for anisotropic effects. Furthermore, using Eq.(A10) there follows that

$$\frac{1}{\Theta_n(\mathbf{r}, t)} = \frac{1}{3} \left( K_{xx}(\mathbf{r}, t) + K_{yy}(\mathbf{r}, t) + K_{zz}(\mathbf{r}, t) \right) = \frac{2}{3} \xi(0) \Phi \left( \frac{m}{2} \tilde{\beta}(\mathbf{r}, t) v^2(\mathbf{r}, t) \right). \quad (\text{A17})$$

Conserving only this contribution in Eq.(A14), linearizing in  $\mathbf{v}(\mathbf{r}, t)$  all expressions, say, the case of a low density flux, assuming a good thermal contact between system and reservoir, such that  $\beta(\mathbf{r}, t) \simeq \beta_R$ , and small amplitude movement, namely  $n(\mathbf{r}, t) \simeq n$ , we are left with a typical Maxwell-type contribution

$$\mathbf{J}_n(\mathbf{r}, t) \simeq -\mathbf{I}_n(\mathbf{r}, t)/\Theta_n, \quad (\text{A18})$$

where

$$\frac{1}{\Theta_n} = \sqrt{\frac{\pi}{2}} n_R \beta_R^{3/2} \sqrt{\frac{M}{m(m+M)}} \xi(0). \quad (\text{A19})$$

## APPENDIX B: ENERGY AND MOMENTUM RELAXATION, EQS.(47) AND (48)

The collision integrals are in this case given by

$$J_j^{(2)}(t) = \left( \frac{1}{i\hbar} \right)^2 \int_{-\infty}^t dt' e^{\epsilon(t'-t)} \text{Tr} \left\{ \left[ \hat{H}'(t')_0, \left[ \hat{H}', \hat{A}_j \right] \right] \bar{\rho}(t, 0) \right\}, \quad (\text{B1})$$

where  $\hat{A}_1 \equiv \hat{H}_e$  for energy and  $\hat{A}_2 \equiv \mathbf{P}$  for momentum, and  $\hat{H}'$  is Fröhlich electron-phonon interaction; subindex nought indicates time dependence in interaction representation. These operators are

$$\hat{H}_e = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m^*} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}, \quad (\text{B2})$$

$$\hat{H}' = \sum_{\mathbf{k}\mathbf{q}} \mathcal{C}_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}} \left( b_{\mathbf{q}} + b_{-\mathbf{q}}^\dagger \right), \quad (\text{B3})$$

$$\mathbf{P} = \sum_{\mathbf{k}} \hbar \mathbf{k} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}, \quad (\text{B4})$$

where  $c_{\mathbf{k}}$  ( $c_{\mathbf{k}}^\dagger$ ) are annihilation (creation) operators of electrons in band state  $\mathbf{k}$ , and the effective mass approximation is taken;  $b_{\mathbf{q}}$  ( $b_{-\mathbf{q}}^\dagger$ ) are annihilation (creation) operator of LO phonons in mode  $\mathbf{q}$ , and the matrix element in Fröhlich interaction is

$$\mathcal{C}_{\mathbf{q}} = -i \frac{\alpha^{1/2}}{q}, \quad (\text{B5})$$

$\alpha$  being Fröhlich coupling constant.

After some calculation one arrives at the results that

$$J_E^{(2)}(t) = \frac{2\pi}{\hbar} \sum_{\mathbf{k}\mathbf{q}} |\mathcal{C}_{\mathbf{q}}|^2 (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \left\{ \left( \nu_{\mathbf{q}}(t) + 1 \right) f_{\mathbf{k}}(t) \left( 1 - f_{\mathbf{k}+\mathbf{q}}(t) \right) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \hbar \omega_{\mathbf{q}}) \right. \\ \left. - \nu_{\mathbf{q}}(t) f_{\mathbf{k}}(t) \left( 1 - f_{\mathbf{k}+\mathbf{q}}(t) \right) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \hbar \omega_{\mathbf{q}}) \right\}, \quad (\text{B6})$$

$$J_{\mathbf{P}}^{(2)}(t) = \frac{2\pi}{\hbar} \sum_{\mathbf{k}\mathbf{q}} |\mathcal{C}_{\mathbf{q}}|^2 \hbar \mathbf{q} \left\{ \left( \nu_{\mathbf{q}}(t) + 1 \right) f_{\mathbf{k}}(t) \left( 1 - f_{\mathbf{k}+\mathbf{q}}(t) \right) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \hbar \omega_{\mathbf{q}}) \right. \\ \left. - \nu_{\mathbf{q}}(t) f_{\mathbf{k}}(t) \left( 1 - f_{\mathbf{k}+\mathbf{q}}(t) \right) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \hbar \omega_{\mathbf{q}}) \right\}, \quad (\text{B7})$$

where, in a nondegenerate-like limit acceptable in the usual experimental conditions

$$f_{\mathbf{k}}(t) = A(t) \exp \left\{ -\beta(t) \frac{\hbar^2}{2m^*} (\mathbf{k} - \mathbf{k}_D)^2 \right\}, \quad (\text{B8})$$

a shifted Maxwell-Boltzmann-like instantaneous distribution, with  $\hbar \mathbf{k}_D = m \mathbf{v}$ ,  $\mathbf{P} = n \mathbf{v}$ ,  $A(t)$  ensures the normalization to  $N$ ,  $\omega_0$  is the LO phonons dispersionless frequency (Einstein model), and [cf. Eq.(54)]

$$\nu_{\mathbf{q}}(t) = \left[ \exp \{ \beta_{LO}(t) \hbar \omega_o \} - 1 \right]^{-1}. \quad (\text{B9})$$

It can be noticed that Eqs.(B6) and (B7) are of the form of the Golden Rule of Quantum Mechanics averaged over the nonequilibrium ensemble. Performing the integrations one arrives to the results presented in Eqs.(47) and (48).

---

[1] A. R. Vasconcellos, J. G. Ramos, and R. Luzzi, preceding article.

- [2] R. Luzzi, A. R. Vasconcellos, J. Casas-Vazquez, and D. Jou, *Physica A* **234**, 699 (1997); *J. Chem. Phys.* **107**, 7383 (1997).
- [3] J. Casas-Vazquez and D. Jou, *Rep. Prog. Phys.* **66**, 1937 (2003).
- [4] R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, *Statistical Foundation of Irreversible Thermodynamics* (Teubner-BertelsmannSpringer, Stuttgart, Germany, 2000); also *Rivista Nuovo Cimento* **24**, 1 (2001).
- [5] R. E. Nettleton, *Can. J. Phys.* **72**, 106 (1994).
- [6] D. Jou, J. Casas-Vazquez, J. R. Madureira, A. R. Vasconcellos, and R. Luzzi, *J. Chem. Phys.* **116**, 1571 (2002); *J. R. Madureira, J. Chem. Phys.* **120**, 7526 (2004).
- [7] J. C. Maxwell, *Phil. Trans. Roy. Soc. (London)* **157**, 49 (1867).
- [8] D. Jou, J. Casas-Vazquez, and G. Lebon, *Extended Irreversible Thermodynamics* (Springer, Berlin, Germany, third enlarged edition, 2002)
- [9] A. C. Algarte, A. R. Vasconcellos, and R. Luzzi, *Phys. Stat. Sol. (b)* **173**, 487 (1992).
- [10] C. G. Rodrigues, A. R. Vasconcellos, and R. Luzzi, *Transp. Theory Stat. Phys.* **29**, 733 (2000).
- [11] R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, *Predictive Statistical Mechanics: A Nonequilibrium Ensemble Formalism* ( Kluwer Academic, Dordrecht, The Netherlands, 2002).
- [12] M. Abramovitz and I. Stegun, *Handbook of Mathematical Functions* (Dover, New York, USA, 1970).
- [13] E. Conwell, *High Field Transport in Semiconductors* in Solid State Physics Series, Suppl. **9**, 1-293 (Academic, New York, USA, 1967).
- [14] S. J. Pearson, Editor, articles in *GaN and Related Materials*, in the Series Optoelectronic Properties of Semiconductors and Superlattices (Gordon and Breach, New York, USA, 1997).
- [15] C. Hilsum, *Proc. IRE* **52**, 185 (1962).
- [16] D. E. Bolger, J. Franks, and J. Gordon, in *Proceedings of the International Symposium on GaAs*, (The Institute of Physics and the Physical Society, London, 1967).
- [17] H. G. B. Hicks and D. F. Manley, *Solid State Commun.* **7**, 1463 (1969).
- [18] D. L. Rode and S. Knight, *Phys. Rev. B* **3**, 2534 (1971).
- [19] N. S. Mansour, L. F. Eastman, U. V. Bahpkar, and M. S. Shour, *J. Appl. Phys.* **77**, 2834 (1995).
- [20] B. E. Foutz, K. W. Kim, and M. A. Littlejohn, *Appl. Phys. Lett.* **70**, 2849 (1997).
- [21] C. G. Rodrigues, A. R. Vasconcellos, V. N. Freire, and R. Luzzi, *Transport Properties of*

Polar Semiconductors in Doped GaAs and III-N Compounds: A Comparison, IFGW-Unicamp Internal Report, and future publication.

- [22] J. G. Ramos, A. R. Vasconcellos, and R. Luzzi, J. Chem. Phys. **112**,2692 (2000).
- [23] T. Dedeurwaerdere, J. Casas-Vazquez, D. Jou, and G. Lebon, Phys. Rev. E **53**, 498 (1996).
- [24] J. R. Madureira,, A. R. Vasconcellos, R. Luzzi, and L. Lauck, Phys. Rev. E **57**, 3637 (1998).
- [25] J. R. Madureira, J. Math. Phys. **41**, 5381 (2000).
- [26] L. Lauck, A. R. Vasconcellos, and R. Luzzi, Physica A **168**, 789 (1990).

## FIGURE CAPTIONS

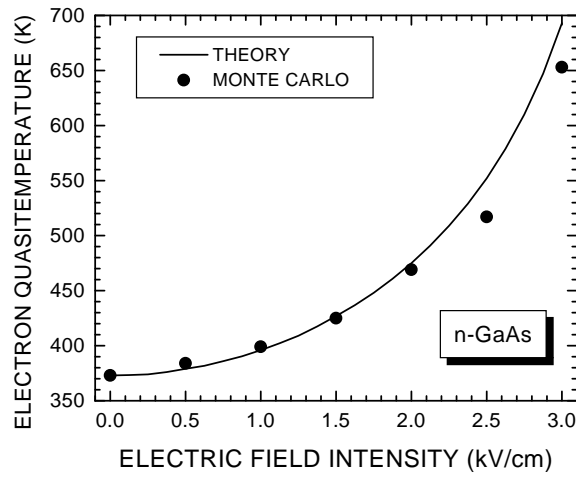


FIG. 1: The electron quasitemperature *vs.* the electric field intensity, in the steady state of *n*-GaAs, comparing the results of the NESEF-based kinetic theory with a Monte Carlo simulation (full circles from ref.[15]).

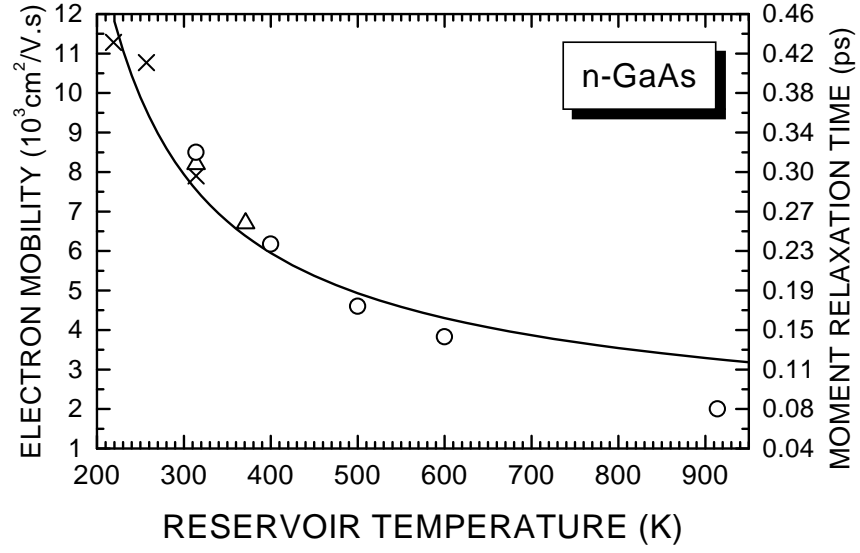


FIG. 2: Electron mobility (and momentum relaxation time) in  $n$ -GaAs for different values of the reservoir temperature, comparing the results of the NESEF-based kinetic theory with experimental data (up triangle from Ref.[14],  $\times$  from Ref.[17], empty circles from Ref.[18]).

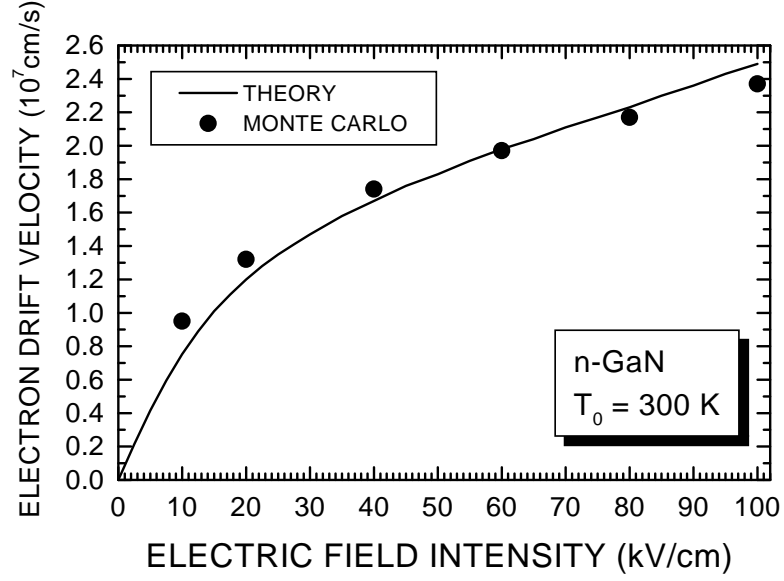


FIG. 3: Electron-drift velocity *vs.* electric field intensity in *n*-GaN, comparing the results of the NESEF-based kinetic theory with a Monte Carlo simulation (Full circle from Ref.[19]), with  $T_0 = 300K$ .

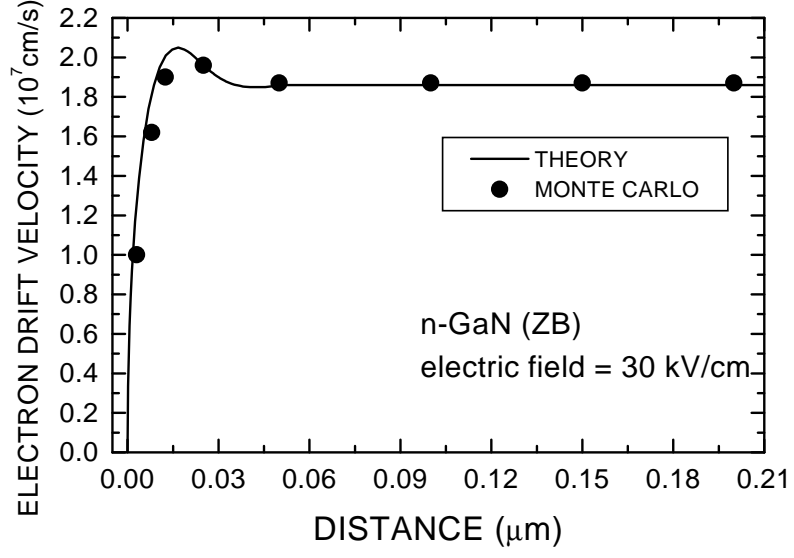


FIG. 4: Evolution of the electron-drift velocity in  $n$ -GaN in terms of the travelled distance, comparing the results of the NESEF-based kinetic theory with a Monte Carlo simulation (Full circles from Ref.[20]): zincblende  $n$ -GaN for an electric field intensity 30kV/cm and  $T_0 = 300K$ .